Reg.No. \_\_\_\_\_\_\_\_\_\_\_\_



**End Semester Examination – Nov/Dec - 2017**

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| **Code :** | **15PH3009** | **Duration :** | **3hrs** |
| **Sub. Name :** | **ATOMIC AND MOLECULAR SPECTROCOPY** | **Max. marks :** | **100** |

**ANSWER ALL QUESTIONS (5 x 20 = 100 Marks)**

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| **Q. No.** | **Sub Div.** | **Questions** | **Course**  **Outcome** | **Marks** |
| 1. | a. | Differentiate UPES and XPES based on principle of working. | CO1 | 4 |
| b. | When 40.81 eV radiation is used to produce photoelectron spectra of neon, photoelectrons of kinetic energy 19 eV have been emitted. Evaluate the ionization energy of these electrons in kJ mol-1. (1 eV= 9.635 x 104 J/mol) | CO3 | 4 |
| c. | Outline the construction and working of photoelectron spectroscopy and discuss how the binding energy is used in finding the oxidation state of an element. | CO2 | 12 |
| (OR) | | | | |
| 2. | a. | List the four different quantum numbers and state what is the function of each. | CO2 | 4 |
| b. | The orbital angular momentum of an electron in a hydrogen like atom is 1.3115 x 10-23 J/T. Justify the state of the electron. | CO2 | 4 |
| c. | Discuss the energies of atomic orbitals for a hydrogen atom spectrum. | CO2 | 12 |
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| 3. | a. | Mention the different spectroscopy techniques associated with the different regions of the electromagnetic spectrum bringing out the nature of transitions involved. | CO1 | 4 |
|  | b. | The first line in the rotation spectrum of carbon monoxide has a frequency of 3.8424 cm-1. Calculate the rotational constant and hence the C-O bond length in carbon monoxide. Avagadro number is 6.022 x 1023 / mol. | CO1 | 4 |
|  | c. | With a neat sketch on energy level diagram, discuss the allowed rotational energies of a rigid diatomic molecule. | CO1 | 12 |
| (OR) | | | | |
| 4. | a. | Illustrate the fundamental vibrations of a H2O molecule with neat sketch? | CO1 | 4 |
|  | b. | The frequency of OH stretching vibration in CH3OH is 3300 cm-1. Estimate the frequency of OD stretching vibration in CH3OD. | CO1 | 4 |
|  | c. | Imagine that the molecule HCl undergoes a simple harmonic vibration. In that case, discuss the vibrational energy levels and transitions between them using FTIR spectroscopy. | CO1 | 12 |
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| 5. | a. | Differentiate Raman and Rayleigh scattering. | CO1 | 4 |
|  | b. | Irradiation of carbon tetrachloride by 4358 Å radiation gives Raman lines at 4400 Å. Calculate the Raman shift in cm-1. | CO1 | 4 |
|  | c. | Discuss the pure rotational Raman spectra of linear diatomic molecule. | CO1 | 12 |
| (OR) | | | | |
| 6. | a. | List the factors that affect the width of spectral lines? | CO3 | 4 |
|  | b. | Explain the reasons behind the changes in intensity of spectral lines. | CO3 | 4 |
|  | c. | Write in detail, the instrumentation part of FTIR spectroscopy with neat sketches. | CO3 | 12 |
| 7. | a. | State the selection rule for Raman Scattering. | CO1 | 4 |
|  | b. | With which type of spectroscopy would one observe the pure rotation spectrum of H2? If the bond length of H2 is 0.07417 nm, what would be the spacing of lines in the spectrum? | CO1 | 4 |
|  | c. | Show how the classical theory uses the concept of molecular polarizability to interpret the Raman Effect. | CO1 | 12 |
| (OR) | | | | |
| 8. |  | The first stokes line in the rotational Raman Spectrum of 14N15N is observed at 11.5416 cm-1. i. What is its B value? ii. Calculate its bond length. iii. Would there be an intensity alteration in the spectrum of 14N15N? iv. Would 14N15N show a rotational spectrum? | CO2 | 20 |
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|  | | **Compulsory**: |  |  |
| 9. | a. | State the Franck-Condon Principle. | CO1 | 4 |
|  | b. | Discuss the intensity of Vibrational-Electronic Spectra: the Franck-Condon Principle. | CO2 | 16 |

ALL THE BEST